Error Estimation for Nonlinear Reduced Basis Methods based on Empirical Operator Interpolation

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Outline

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Scenario:

DISCRETE operators $\mathcal{L}_h(\boldsymbol{\mu}) : \mathcal{V}_h \to \mathcal{W}_h$
for PARAMETER vectors $\boldsymbol{\mu} \in \mathcal{M} \subset \mathbb{R}^p$.

Goals:

- Linearization
- Parameter separation
- Fréchet derivatives
- A posteriori error estimation

Discrete parametrized operators $\mathcal{L}_h(\boldsymbol{\mu}) : \mathcal{V}_h \to \mathcal{W}_h$

Definition: discrete function space $\mathcal{W}_h$

- Hilbert-space $\mathcal{W}_h \subset L^\infty(\Omega)$
- has basis functions $\{\psi_i\}_{i=1}^H, \psi_i \in \mathcal{W}_h$ and
- DOF functionals $\Sigma_h := \{\tau_i\}_{i=1}^H$, with $\tau_i : \mathcal{W}_h \to \mathbb{R}$, such that
- for all $u_h \in \mathcal{W}_h : u_h = \sum_{i=1}^H \tau_i(u_h)\psi_i$

Empirical operator interpolation

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Empirical operator interpolation

Discrete parametrized operators $\mathcal{L}_h(\boldsymbol{\mu}) : \mathcal{V}_h \to \mathcal{W}_h$

Ingredients

- "Trained" set: $\mathcal{X} := \{\mathcal{L}_h(\boldsymbol{\mu})\,[u_h(\boldsymbol{\mu})]\,;\boldsymbol{\mu} \in \mathcal{M}\}$
- POD- or interpolation basis: $\{q_m\}_{m=1,\dots,M}$
- Interpolation DOFs: $\left\{\tau_m^{EI}\right\}_{m=1}^{M}$, with $\tau_m^{EI} \in \Sigma_h$

References: (B.Haasdonk, M.Ohlberger, G.Rozza, 2008) and (M.Drohmann, B.Haasdonk, M.Ohlberger, 2012)

Interpolation is based on the simple idea:

$$\mathcal{I}_M\left[\mathcal{L}_h\right] := \mathcal{I}_M\left[\mathcal{L}_h\left[\cdot\right]\right]$$

Empirical operator interpolation: Properties

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- Interpolants of Fréchet DERIVATIVES efficiently computable

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- Invariance of "linear operator properties":
  - especially global and local conservation of finite volume operators

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- Interpolants of Fréchet DERIVATIVES efficiently computable
- INVARIANCE of "linear operator properties":
  - especially global and local conservation of finite volume operators
- Computationally equivalent to DEIM

For $v_h \in \mathcal{X}$

the interpolation error $\|v_h - \mathcal{I}_M[v_h]\|_{L^\infty}$ can be bounded:

- A priori under assumption of possible exponential convergence (Maday et al, 2009)
- A posteriori under assumption of exactness for $M + M'$ interpolation basis functions.
- Globally, i.e. for all $\mu \in \mathcal{M}$ (Barrault et al, 2004) and (Eftang et al., 2010)
- With respect to its best approximation

$$\min_{w_h \in \mathrm{span}\{q_m\}_{m=1}^M} \|w_h - v_h\|_{L^\infty}$$

via computable Lebesgue constant $\Lambda_M \leq 2^M - 1$. (Barrault et al, 2004)

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Scalar Evolution Equation

Analytical Formulation

For $\boldsymbol{\mu} \in \mathcal{M} \subset \mathbb{R}^p$, find $u : [0, T_{\max}] \to \mathcal{W} \subset L^2(\Omega)$, s.t.

$$u(0) = u_0(\boldsymbol{\mu}), \qquad \partial_t u(t) - \mathcal{L}(\boldsymbol{\mu})\,[u(t)] = 0$$

plus (parameter dependent) boundary conditions.

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Discretization (implicit/explicit with Newton scheme)

For $\boldsymbol{\mu} \in \mathcal{M}$ find $\{u_h\}_{k=0}^{K} \subset \mathcal{W}_h \subset \mathcal{W}$, s.t.

$$u_h^0 := \mathcal{P}_h\left[u_0(\boldsymbol{\mu})\right], \qquad u_h^{k+1} := u_h^{k+1,\nu_{\max}(k)}$$

with Newton iteration

$$u_h^{k+1,0} := u_h^k, \qquad u_h^{k+1,\nu+1} := u_h^{k+1,\nu} + \delta_h^{k+1,\nu+1},$$

$$\left(\mathrm{Id} + \Delta t \mathbf{D} I|_{u_h^{k+1,\nu}}\right)\left[\delta_h^{k+1,\nu+1}\right] = u_h^k - u_h^{k+1,\nu} - \Delta t \left(I\left[u_h^{k+1,\nu}\right] + E\left[u_h^k\right]\right).$$

Reduced basis scheme (DHO, 2012)

Reduced simulation (implicit/explicit with Newton scheme)

For $\boldsymbol{\mu} \in \mathcal{M}$ find $\left\{u_h^k(\boldsymbol{\mu})\right\}_{k=0}^K \subset \mathcal{W}_h \subset \mathcal{W}_h$, such that

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$$\mathcal{L}_{\mathrm{red},I/E} := \mathcal{P}_{\mathrm{red}} \circ \mathcal{I}_M \circ I/E$$

A posteriori error estimator (DHO, 2012)

Estimator

$$\left\| u_h^k(\boldsymbol{\mu}) - u_{\mathrm{red}}^k(\boldsymbol{\mu}) \right\| \leq \eta_{N,M,M'}^k(\boldsymbol{\mu})$$

Two main contributions:

- Projection error on $\mathcal{W}_{\mathrm{red}}$ (exactly computable!)
- Empirical interpolation error ($M + M'$ trick)

Plus: "Lipschitz" properties:

- $\|u - v + \Delta t \mathcal{L}_I[u] - \Delta t \mathcal{L}_I[v]\|_{\mathcal{W}_h} \geq \frac{1}{C_{I,\Delta t}} \|u - v\|_{\mathcal{W}_h}$
- $\|u - v - \Delta t \mathcal{L}_E[u] + \Delta t \mathcal{L}_E[v]\|_{\mathcal{W}_h} \leq C_{E,\Delta t} \|u - v\|_{\mathcal{W}_h}$

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EI basis generation

EI-Greedy

- With interpolation error $\varepsilon_M(u_h) := \|\mathcal{I}_M[u_h] - u_h\|_{L^\infty}$,
- iteratively search for
- collateral reduced basis functions $q_M := \arg\max_{u_h \in \mathcal{X}_{\text{train}}} \varepsilon_{M-1}(u_h)$ and
- Interpolation DOFs $\tau_m^{EI} := \arg\max_{\tau \in \Sigma_h} |\tau[\mathcal{I}_{M-1}[q_M]] - \tau[q_M]|$.

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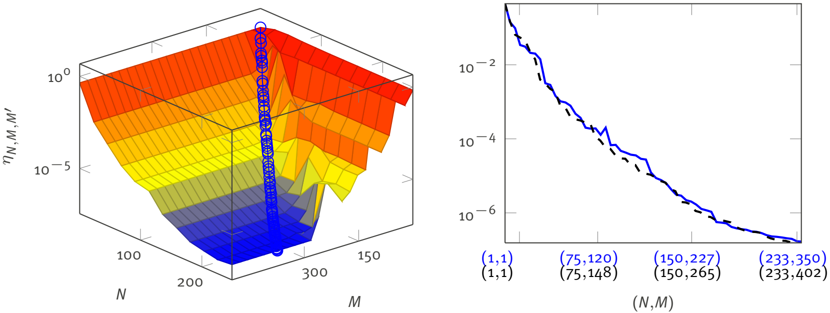
Variants:

- only search for interpolation DOFs (POD-DEIM, GNAT)
- use different (RB)-error (PODEI-Greedy, T.Tonn)

Coupling of basis spaces



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Coupled systems

Solve for $(u_h^1, \ldots, u_h^I) \in \mathcal{V}_h := \mathcal{V}_h^1 \times \ldots \times \mathcal{V}_h^I$

Discretization

$$\mathcal{L}_h^1 \left[(u_h^1, \ldots, u_h^I) \right] = 0$$

$$\vdots \qquad \qquad \vdots$$

$$\mathcal{L}_h^J \left[(u_h^1, \ldots, u_h^I) \right] = 0$$

with discrete operators $\mathcal{L}_h^j : \mathcal{V}_h \to \mathcal{W}_h^j, j = 1, \ldots, J$.

Coupled evolution systems

Solve for $(u_h^1, \ldots, u_h^I) \in \mathcal{V}_h := \mathcal{V}_h^1 \times \ldots \times \mathcal{V}_h^I$

Discretization

$$\left(\frac{\partial u_h^1}{\partial t}\right) + \mathcal{L}_h^1 \left[(u_h^1, \ldots, u_h^I)\right] = 0$$

$$\vdots \qquad \vdots$$

$$\mathcal{L}_h^J \left[(u_h^1, \ldots, u_h^I)\right] = 0$$

+initial condition

with discrete operators $\mathcal{L}_h^j : \mathcal{V}_h \to \mathcal{W}_h^j, j = 1, \ldots, J$.

How to reduce with RB method?

(A) Generate reduced bases $\Phi^1_{N_1} \subset \mathcal{V}^1_h, \dots, \Phi^I_{N_I} \subset \mathcal{V}^I_h$
and empirical operator interpolants $\mathcal{I}^1_{M_1}\left[\mathcal{L}^1_h\right], \dots, \mathcal{I}^J_{M_J}\left[\mathcal{L}^J_h\right]$

(B) Generate reduced basis $\Phi_N \subset \mathcal{V}_h$
and empirical operator interpolant $\mathcal{I}_M\left[\left(\mathcal{L}^1_h, \dots, \mathcal{L}^J_h\right)^t\right]$ (equivalent to scalar case)

(C) "Something between (A) and (B)"

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Assumption: $M_1 + \ldots + M_I < M$ and $N_1 + \ldots + N_I < N$

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$\Rightarrow$ Heuristic algorithms for optimal basis sizes

A posteriori error estimator (DHO, 2012)

Estimator

$$\left\| u_h^k(\boldsymbol{\mu}) - u_{\mathrm{red}}^k(\boldsymbol{\mu}) \right\| \leq \eta_{N,M,M'}^k(\boldsymbol{\mu})$$

Two main contributions:

- Projection error on $\mathcal{W}_{\mathrm{red}}$ (exactly computable!)
- Empirical interpolation error ($M + M'$ trick)

Plus: "Lipschitz" properties:

- $\|u - v + \Delta t \mathcal{L}_I[u] - \Delta t \mathcal{L}_I[v]\|_{\mathcal{W}_h} \geq \frac{1}{C_{I,\Delta t}} \|u - v\|_{\mathcal{W}_h}$
- $\|u - v - \Delta t \mathcal{L}_E[u] + \Delta t \mathcal{L}_E[v]\|_{\mathcal{W}_h} \leq C_{E,\Delta t} \|u - v\|_{\mathcal{W}_h}$

Theorem (A posteriori error estimator)

Assumptions:

- *Operators fulfill "Lipschitz" properties:*
  - $\|u - v + \Delta t \mathcal{L}_I[u] - \Delta t \mathcal{L}_I[v]\|_{\mathcal{W}_h} \geq \frac{1}{C_{I,\Delta t}} \|u - v\|_{\mathcal{W}_h}$
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- *M'-trick: Empirical interpolations exact for larger CRB space $\mathcal{W}_{M+M'}$ and* $\mathcal{P}_h[u_0(\boldsymbol{\mu})] \in \mathcal{W}_{\mathrm{red}}$

A posteriori error estimator

Theorem (A posteriori error estimator cont.)

Assumptions:

- *Operators fulfill "Lipschitz" properties:*
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- *M'-trick: Empirical interpolations exact for larger CRB space $\mathcal{W}_{M+M'}$ and* $\mathcal{P}_h[u_0(\boldsymbol{\mu})] \in \mathcal{W}_{\text{red}}$

Then:

$$\left\| u^k_{\text{red}}(\boldsymbol{\mu}) - u^k_h(\boldsymbol{\mu}) \right\| \leq \eta^k_{N,M}(\boldsymbol{\mu})$$

with

$$\eta_{N,M}(\boldsymbol{\mu}) := \sum_{i=0}^{k-1} C^{k-i+1}_{I,\Delta t} C^{k-i}_{E,\Delta t} \left(\left\| R^{k+1}_{I+E,M}(\boldsymbol{\mu}) \right\| + \left\| \Delta t R^{k+1}(\boldsymbol{\mu}) \right\| + \varepsilon^{New} \right)$$

Theorem (A posteriori error estimator)

Then:

$$\left\| u_{\mathrm{red}}^{k}(\boldsymbol{\mu}) - u_{h}^{k}(\boldsymbol{\mu}) \right\| \leq \eta_{N,M}^{k}(\boldsymbol{\mu})$$

with

$$\eta_{N,M}(\boldsymbol{\mu}) := \sum_{i=0}^{k-1} C_{I,\Delta t}^{k-i+1} C_{E,\Delta t}^{k-i} \left(\left\| R_{I+E,M}^{k+1}(\boldsymbol{\mu}) \right\| + \left\| \Delta t R^{k+1}(\boldsymbol{\mu}) \right\| + \varepsilon^{New} \right)$$

The residuals $R_{*,M}$ measure the empirical interpolation error, e.g.

$$R_{*,M}^{k+1,\nu} := \sum_{m=M}^{M+M'} l_m^{*} \left[u_{\mathrm{red}}^{k+1,\nu} \right] \xi_m$$

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Conclusion

- Model order reduction of general parametrized evolution schemes
- with reduced basis methods and empirical operator interpolation
- specialized reduced basis spaces and empirical interpolation Dofs desirable

Outlook

Conclusion

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Future work

- Parametrization of Two–Phase–Flow example
- Rigorous error control of reduced data

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